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Resolving model parameter values from carbon and nitrogen stock measurements in a wide range of tropical mature forests using nonlinear inversion and regression trees

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ABSTRACT

Objectively assessing the performance of a model and deriving model parameter values from observations are critical and challenging in landscape to regional modeling. In this paper, we applied a nonlinear inversion technique to calibrate the ecosystem model CENTURY against carbon (C) and nitrogen (N) stock measurements collected from 39 mature tropical forest sites in seven life zones in Costa Rica. Net primary productivity from the Moderate-Resolution Imaging Spectroradiometer (MODIS), C and N stocks in aboveground live biomass, litter, coarse woody debris (CWD), and in soils were used to calibrate the model. To investigate the resolution of available observations on the number of adjustable parameters, inversion was performed using nine setups of adjustable parameters. Statistics including observation sensitivity, parameter correlation coefficient, parameter sensitivity, and parameter confidence limits were used to evaluate the information content of observations, resolution of model parameters, and overall model performance. Results indicated that soil organic carbon content, soil nitrogen content, and total aboveground biomass carbon had the highest information contents, while measurements of carbon in litter and nitrogen in CWD contributed little to the parameter estimation processes. The available information could resolve the values of 2–4 parameters. Adjusting just one parameter resulted in under-fitting and unacceptable model performance, while adjusting five parameters simultaneously led to over-fitting. Results further indicated that the MODIS NPP values were compressed as compared with the spatial variability of net primary production (NPP) values inferred from inverse modeling. Using inverse modeling to infer NPP and other sensitive model parameters from C and N stock observations provides an opportunity to utilize data collected by national to regional forest inventory systems to reduce the uncertainties in the carbon cycle and generate valuable databases to validate and improve MODIS NPP algorithms.

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1. Introduction

Numerical models are frequently being used to characterize and predict landscape processes and consequences. Most landscape modeling efforts rely on deploying classic plot-scale models in space using various spatial databases as input data and driving forces (Reiners et al., 2002; Liu et al., 2004a,b). One of the main challenges of this approach is the difficulty in quantifying the spatial variability of model parameters. Conventionally, one or multiple lookup tables are often used to prescribe the variability of some sensitive parameters across various strata (usually by land cover, plant functional type, or biome) in the study area (Parton et al., 1987). In this case, each stratum will have a unique set of parameter values. Although this approach deals with parameter variability to a certain degree, it ignores the impacts of additional environmental factors on parameter variability. For example, some model parameters (e.g., soil hydraulic conductivity and gross primary productivity) are often different among different sites of the same ecosystem types. Because of the variability of parameter values, model calibration is often needed to find the optimal set of parameter values for any given site. For modeling processes over large areas, it is ideal that spatially explicit parameter surfaces or fields are available or can be generated. Otherwise, the simulated spatial patterns might be flawed or even incorrect.

Generating parameter surfaces requires the following key elements:

1. Field measurements collected from many sites in the study area.
2. A consistent and objective calibration procedure to derive optimal model parameter values from these field measurements.
3. Analysis and quantification of the relationship between parameter values and environmental variables such as precipitation and temperature.
4. Mapping parameter surfaces using the relationships established in previous steps.

In this paper, we will concentrate on the second and the third step, which is most challenging among all these steps. Conventional calibration is done manually, which can be very time-consuming, subjective, and challenging, if multiple constraints need to be considered and satisfied at the same time and the model is to be calibrated on many points in space. Furthermore, the optimal set of parameter values usually could not be reached using the manual approach. To overcome these shortcomings, we in this paper applied a nonlinear inversion technique to calibrate the ecosystem model CENTURY against carbon stock measurements collected from 39 mature tropical forest sites in seven life zones in Costa Rica. The number of adjustable parameters that can be resolved by field measurements will be discussed. The usefulness of the nonlinear inversion technique in inferring net primary production (NPP) will be presented and the estimated NPP will be compared with MODIS NPP. The quantitative relationships between parameter values and site factors will be explored using piece-wise regression tree techniques.

2. Methods

2.1. *Study area and field data collection*

As a part of an effort to generate supply functions of carbon sequestration in Costa Rica (Pfaff et al., 2000; Kerr et al., 2003), carbon (C) and nitrogen (N) stocks at the stand level were estimated at 39 mature forest sites spread in six Holdridge life zones (Table 1) in 2000 and 2001 (Fig. 1). The annual precipitation varies from about 1000 to 6000 mm, and annual mean air temperature ranges from 10 to 22 °C across these sites and life zones.

Diameters at breast height of live and dead trees were measured for all the trees in the 100 m × 100 m plots. C stocks in aboveground live biomass and coarse woody debris were then estimated using allometric equations that relate diameter at breast height (DBH) of a tree to its carbon content (Hughes et al., 2002). Carbon stocks on forest floor and in soil were also measured. C and N ratios of aboveground biomass, coarse woody debris, litter, and soils were measured and used to estimate N stocks in these compartments. Soil samples were taken to measure physical and chemical properties including bulk density and texture. Detailed description on field measurements and data processing can be found in Hughes et al. (2002).

2.2. *Net primary production and climate data*

Annual net primary productions (NPP) at these sites were derived from the Moderate-Resolution Imaging Spectroradiometer (MODIS) (http://modis.gsfc.nasa.gov/). MODIS NPP data were at 1 km resolution. In order to minimize the errors introduced by spatial registration of the field plots and frequent cloud cover in Costa Rica, the maximum annual NPP within a 5 km × 5 km window was extracted from the MODIS NPP surface in 2001. This maximum NPP was assumed to represent the annual NPP of the mature forest site and used in model calibration.

Monthly precipitation, maximum, and minimum temperatures are required to run the CENTURY model. Few field sites had weather stations nearby. Surfaces of the long-term means of these climate variables were generated using Kriging and data collected from the network of weather stations in Costa Rica (Waylen et al., 1996). Climate data for each of the study sites were extracted from these surfaces according to their geographic locations.

2.3. *Estimation of mortality rate*

Mortality is an important parameter in all ecosystem models including CENTURY because its magnitude can affect the levels of C and N stocks and fluxes of an ecosystem. To study and simulate the spatial variation of C and N dynamics across life zones, it is necessary to understand and quantify how mortality changes across life zones and which site characteristics are most likely to affect the mortality of the tropical forests. No mortality observations were available for the study sites because reliable estimates require long-term observations and beyond the scope of our study. In

Table 1 – Study sites and their associated Holdridge life zones: Tropical Dry Forest (T-df), Lower Montane Rain Forest (LM-rf), Tropical Moist Forest (T-mf), Premontane Rain Forest (P-rf), Premontane Wet Forest (P-wf), and Tropical Wet Forest (T-wf)

Site ID	Site name	Life zone code	Site ID	Site name	Life zone code
1	Meseta	T-df	21	Kraven	P-rf
2	Pacifica1	T-df	22	Saino	P-rf
3	Pacifica2	T-df	24	OldRoad	P-wf
4	Pacifica3	T-df	25	Mary	P-wf
5	Roedores	T-df	26	Las Alturas	P-wf
7	Bellbird	LM-rf	27	Rodeo3	P-wf
8	Pittier	LM-rf	29	SSO-LaSelva	P-wf
9	Valle	LM-rf	30	Holdridge	P-wf
10	Nuboso	LM-rf	31	La Muerte	P-wf
11	Trinidad	LM-rf	33	Magsasay	T-wf
13	Carara1	T-mf	34	Gallo Pinto	T-wf
14	Carara2	T-mf	35	La Bonita	T-wf
15	Jobada	T-mf	36	Maria Luisa	T-wf
16	Killer	T-mf	37	Osa1	T-wf
17	Puntas Blancas	T-mf	38	Osa2	T-wf
19	Penas Blancas	P-rf	39	Osa3	T-wf
20	Miranda	P-rf			

order to understand the spatial variation of mortality and its relationship to site conditions, we conducted a literature review on previous mortality studies in tropical forests. Results indicated that mortality was not strongly affected by slope (Herwitz and Young, 1994; Matelson et al., 1995; Bellingham and Tanner, 2000), elevation (Carey et al., 1994; Matelson et al., 1995), wind and soil type (Matelson et al., 1995). Drought, on the other hand, was found to have some affect on mortality with smaller trees and shrubs affected more intensely by drought than the larger class of trees and shrubs (Condit et al., 1995). Mortality is affected by tree species (Lang and Knight, 1983; Korning and Balslev, 1994) and tree size (Liberman et al., 1985; Liberman and Liberman, 1987; Korning and Balslev, 1994). The impacts of tree species and size on mortality are demonstrated within individual stands. Their impacts on mature forests at the stand level are not clear.

Because no apparent quantitative relationships were found between mortality rates and site conditions, it is not possible for us to assign site-specific mortality rates to these study sites according to their biotic and abiotic conditions. In this study, the mortality rates were assumed to be the same for all the sites with the average rate of 0.173% biomass y^{-1} derived from the literature above.

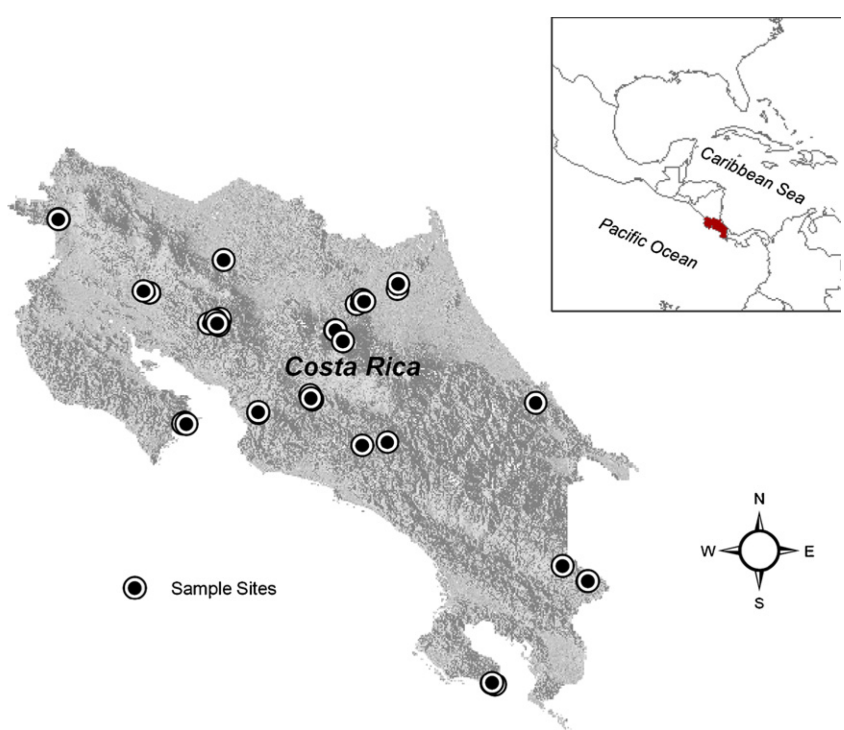

Fig. 1 – Field sites for measuring C and N stocks in mature forests in Costa Rica.

2.4. CENTURY model

The CENTURY model (version 4) was designed to simulate C, N, P, and S cycles in various ecosystems including crops, pastures, forests, and savannas worldwide (Parton et al., 1987; Schimel et al., 1991, 1994; Pan et al., 1998; Liu et al., 1999; Reiners et al., 2002). We have modified and applied the model to simulate the emissions of nitrogen trace gases from soils into the atmosphere in the Atlantic lowlands of Costa Rica (Liu et al., 1999, 2000; Reiners et al., 2002). The main input data of the model include:

1. Climate data: monthly precipitation, monthly maximum temperature, and monthly minimum temperature.
2. Soil data: bulk density, fractions of sand, silt, and clay, and drainage conditions.
3. Biological data: major species or ecosystem type, C:N ratios of plant tissues, mortality, and maximum gross primary productivity.
4. Management practices and disturbances such as land use activities and hurricanes.

Because we dealt with mature forests that had no visible evidence of any disturbances in this study, management and disturbances were not considered in model simulations.

2.5. Nonlinear inversion

2.5.1. Nonlinear inversion and PEST

The goal of nonlinear inversion is to derive a set of model parameter values that minimize the least squares of the weighted residuals (PEST, 2003):

$$\Phi = \min \sum_{i=1}^{m} [w_i(y_i' - y_i)]^2 \qquad (1)$$

where w_i is the weight of ith observation y_i, y_i' is the model simulated value corresponding to the ith observation, and m is the total number of observations. The observation data items that were used at each site for nonlinear inversion are listed in Table 2.

The optimization of (1) was accomplished using the software PEST. PEST takes control of the CENTURY model and runs it as many times as necessary to reach an optimal set of parameter values. PEST calculates the mismatch between the model output and the observation data and then determines the best way, by adjusting the values of model parameters, to correct the mismatch. This process is repeated until the objective function (1) is minimized. The corresponding final set of parameter values are said to be optimal.

2.5.2. Modeling experiment design

What parameter values should be adjusted and what weights should be assigned to different observations are important issues in nonlinear inversion. Only a certain number of parameters can practically be resolved for a given set of observations (Wang et al., 2001). In order to investigate the power of the observations in resolving model parameters, nine separate run batches of the PEST/Century model were preformed. A run batch consisted of running the PEST-CENTURY setup separately at each of the 39 sites. A different set of adjustable, tied, or fixed parameters was assigned to each of the batches, and the combination of parameters for a particular batch was consistent across sites. The combinations of the 11 parameters being adjustable, tied, or fixed in this study are listed in Table 3. These parameters play important roles in carbon cycle simulations in the CENTURY model. Parameters that were adjustable or tied were of significance since their values would be optimized based on the model and the observation data. A parameter is tied with an adjustable parameter using a multiplicative constant. All other parameters of the CENTURY model that were not listed remained fixed in all model runs.

Table 2 – Observed variables that have been used for model calibration and testing

Observation code	Definition
NPP	Net primary production ($g\,C\,y^{-1}$)
ABGC	Carbon in aboveground biomass ($g\,C\,m^{-2}$)
LITTERC	Carbon in litter ($g\,C\,m^{-2}$)
WOODC	Carbon in dead wood ($g\,C\,m^{-2}$)
SOMTC	Soil organic carbon in the top 20 cm layer ($g\,C\,m^{-2}$)
ABGN	Nitrogen in aboveground biomass ($g\,N\,m^{-2}$)
LITTERN	Nitrogen in litter ($g\,N\,m^{-2}$)
WOODN	Nitrogen in dead wood ($g\,N\,m^{-2}$)
SOMTN	Nitrogen in the top 20 cm soil layer ($g\,N\,m^{-2}$)

Weights were assigned to these observations to reflect the magnitudes of the values and the quality of the data (Table 4). For example, because N content is at least 10 times lower than the C content in both vegetation and soils, a weight of 10 or larger would be needed for N values in order to make the contribution of N residuals comparable to that of C residuals in the objective function. Otherwise, the N residuals would be too small numerically to play a role in the objective function as compared with the C residuals, although both kinds of residuals are equally important in judging the success of model calibration. The weights can also be used as an indicator of confidence in data quality or the nature of the data. In our study, we assigned a value of 0.3 as the weight of coarse woody debris (CWD) because CWD measured at any given time might not represent its long-term average, which is really what the CENTURY simulates, because of the erratic nature of tree mortality. Putting too much weight in CWD would force the modeling system to run in a state that might be different from reality. The weights for the observations were changed in different runs to investigate the importance of the observation data on model inversion (Table 4).

2.5.3. Diagnostic and inferential statistics for inverse modeling

Four issues need to be considered for estimating model parameter values: sensitivity of parameters and observations,

Table 3 – Combinations of 11 parameters being adjustable (V), tied (T), or fixed (F) for the nine model run batches

Parameter	ID	Model run batch									Parameter definition
		1	2	3	4	5	6	7	8	9	
dec11	(a)	V	V	V	V	F	T(b)	T(d)	T(d)	F	Maximum surface structural decomposition rate
dec4	(b)	V	V	V	V	F	V	T(d)	T(d)	F	Maximum decomposition rate of soil organic matter with active turnover
dec5	(c)	T(b)	T(b)	T(b)	T(b)	F	T(b)	T(d)	T(d)	F	Maximum decomposition rate of soil organic matter with slow turnover
prdx4	(d)	V	V	V	V	V	V	V	V	V	Maximum gross forest production
decw1	(e)	V	V	V	F	F	F	F	F	F	Maximum decomposition rate constant for dead fine branch
decw2	(f)	T(e)	T(e)	T(e)	F	F	F	F	F	F	Maximum decomposition rate constant for large wood
wooddr2	(g)	V	V	F	F	F	F	F	F	F	Monthly death rate fraction for fine roots
wooddr3	(h)	T(g)	T(g)	F	F	F	F	F	F	F	Monthly death rate fraction for fine branches
wooddr4	(i)	T(g)	T(g)	F	F	F	F	F	F	F	Monthly death rate fraction for large wood
wooddr5	(h)	T(g)	T(g)	F	F	F	F	F	F	F	Monthly death rate fraction for coarse roots
teff2	(k)	—	—	—	—	-	—	—	—	V	Minimum temperature for vegetation growth

The letter in parentheses is the ID of the variable that was tied with.

nonuniqueness of parameter values, parameter uncertainty, and overall model fit. These issues can be addressed using the diagnostic and inferential statistics described in the following subsections.

2.5.3.1. *Parameter sensitivity.* High parameter sensitivity values indicate that these parameters are likely to be easy to estimate by inversion with the observations, while low values are not. In other words, the available observations contain substantial information about parameters with high sensitivity values, less information about those with low sensitivity values.

Since absolute composite sensitivities are not suitable for parameters of different type and magnitude (PEST, 2003), we used the relative composite sensitivities to compare the effects of different parameters on the parameter estimation process. The relative composite sensitivity for a given model parameter, s_i, is obtained by multiplying the parameter's absolute composite sensitivity by the value of the parameter:

$$s_i = \frac{\sqrt{(\underline{J}^t \underline{Q}\underline{J})_{i,i}}}{m}\beta_i \tag{2}$$

where $\underline{J}$ represents the Jacobian matrix, $\underline{Q}$ is the cofactor matrix, β_i is the value of the parameter, and m is the number of observations that have non-zero weights (PEST, 2003). The Jacobian matrix is made up of m rows and n (i.e., the number of adjustable parameters) columns. The elements in the Jacobian matrix are the derivatives of the observations with respect to the adjustable parameters. The cofactor matrix is most often a diagonal matrix with the elements being the squared observation weights. The relative composite sensitivities are used during the parameter estimation process to determine which parameters might be degrading the model

Table 4 – Weights were assigned to observations to reflect the magnitudes of the values and the quality of the data

Parameter	Model run ID								
	1	2	3	4	5	6	7	8	9
NPP	10	10	1	1	1	1	1	10	1
abgc	1	1	1	1	1	1	1	1	1
litterc	1	1	1	1	1	1	1	1	1
woodc	1	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
somtc	1	1	1	1	1	1	1	1	1
abgn	10	10	10	10	10	10	10	10	10
littern	10	10	10	10	10	10	10	10	10
woodn	10	3	3	3	3	3	3	3	3
somtn	10	10	10	10	10	10	10	10	10

The weights were changed in different runs to investigate the importance of the observation data on model inversion.

performance because they lack sensitivity to model outcomes (Poeter and Hill, 1998).

2.5.3.2. *Observation sensitivity*. The composite observation sensitivity of observation δ_j is defined as:

$$\delta_j = \frac{\sqrt{\{\underline{Q}(\underline{JJ}^T)\}_{j,j}}}{n} \tag{3}$$

Therefore, the composite observation sensitivity of observation j is the magnitude of jth row of the Jacobian matrix multiplied by the weight of the observation, and then divided by the number of adjustable parameters (PEST, 2003). It is thus a measure of the sensitivity of the observation to all parameters in the parameter estimation process. High observation sensitivity suggests high information content and therefore contributes more to the parameter estimation process.

2.5.3.3. *Parameter correlation coefficient matrix*. Parameter correlation coefficients suggest whether the estimated parameter values are likely to be unique. High correlation coefficients between parameters are indicative of a high degree of uncertainty (i.e., wide confidence intervals) in the parameter estimation process. The parameter correlation coefficient matrix is symmetric with one row and column for each of the adjustable parameters. Fixed and tied parameters are not included in the matrix. The elements of the correlation coefficient matrix are calculated as

$$\rho_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}} \tag{4}$$

where σ_{ij} represents the element at the ith row and jth column of the covariance matrix (PEST, 2003). The elements along the diagonal of the correlation coefficient matrix are always 1. All other elements in the matrix are between 1 and −1. Each of the elements in the matrix represents the correlation between the parameter in that row and that column. The closer the values off the diagonal are to 1 or −1 the more correlated the two parameters are, and the observations used in the inversion are not likely to be able to uniquely resolve these parameters.

2.5.3.4. *Parameter uncertainty*. Parameter uncertainty can be approximately quantified using linear confidence intervals (Poeter and Hill, 1998):

$$\beta_j \pm t_{(f,1.0-\alpha/2)}\upsilon_j \tag{5}$$

where β_j and υ_j are the adjustable parameter value and its associated standard deviation, respectively, and $t_{(f,1.0-\alpha/2)}$ is the Student-t statistic for f degree of freedom and a significance level of α.

Narrow intervals indicate greater precision. If the model accurately represents the system, the intervals also suggest the likely accuracy of the estimate. If the confidence interval includes no realistic parameter values, the unrealistic parameter estimate is likely to suggest problems with the model or observations. If the confidence interval includes unrealistic parameter values, it is usually not clear whether there is a problem with the model or the observations.

2.5.3.5. *Goodness of overall model fit*. Two methods were used to assess the goodness of model fit across sites. We first visually analyzed the patterns of the residuals. Good model fit would produce small residuals that are close to zero. To assess model fit more objectively, a linear regression between observed and simulated values for each of the variables was developed. A successful model fit would satisfy all the following conditions:

1. The linear regression is significant at $\alpha = 0.01$.
2. The slope of the regression is not significantly different from 1 at $\alpha = 0.005$.
3. The intercept of the regression is not significantly different from 0 at $\alpha = 0.005$.

2.6. Modeling model parameters

The values of model parameters might vary with precipitation, temperature, drainage condition, and other site characteristics. It is important to understand and able to predict the changes of model parameter values in space and time in order to apply models to unobserved territories. Often, the variability of parameter values can only be represented by lookup tables due to limited understanding of the controlling factors. In this study, the rule-based data-mining tool Cubist [http://www.rulequest.com/cubist-info.html] was used to develop empirical models for the variable parameters from the above inversed parameter values.

Both a single model and a committee model were created for each parameter, and the better model was selected for prediction. The committee approach created several single models (i.e., a committee) for any given parameter, and the predicted value of the parameter was given by the average of the predicted values of all the single models in the committee. The independent variables for the Cubist piece-wise regression were precipitation, minimum temperature, mean temperature, maximum temperature, life zone, and elevation at each site. In order to account for dependence of a parameter on any other parameters, model parameters were included as independent variables.

To select the best possible set of models for all the parameters, we have to consider the determination coefficients, relative errors, and precedence of the models. Precedence is important when two or more parameters are significantly related. For example, if parameter A is correlated with parameter B and A can be better predicted without knowing B than otherwise (e.g., judged by their determination coefficients and relative errors), then A has a higher precedence than B, and B should not be included in the model of A.

3. Results

3.1. Observation sensitivity

Observation sensitivities for all 9 run batches indicated several patterns (Fig. 2). First, sensitivities of a given observation within a given run batch varied 1–5 magnitudes across sites, indicating that the information contained in an observation varied from site to site. Second, the sensitivities of differ-

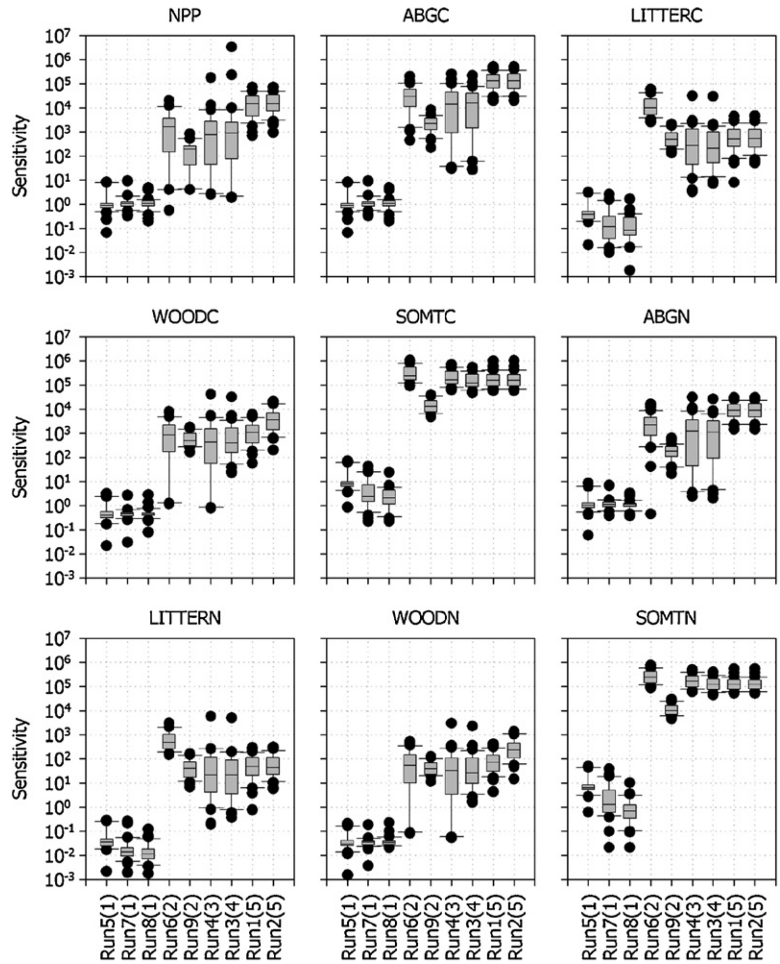

Fig. 2 – Observation sensitivities from 9 model run batches. The boundary of the box closest to zero indicates the 25th percentile, a line within the box marks the median, and the boundary of the box farthest from zero indicates the 75th percentile. Whiskers (error bars) above and below the box indicate the 90th and 10th percentiles.

ent observations varied greatly and the medians differed several magnitudes. For all these nine run batches, SOMTC, SOMTN, and ABGC had the highest sensitivities, suggesting they contained more information that contributed to the determination of the adjustable parameters than other observations. Meanwhile, LITTERN, WOODN, and LITTERC had the lowest sensitivities and contributed lesser to the parameter estimation process than other variables. Third, observation sensitivities varied among model run batches, reflecting the impacts of different combinations of adjustable parameters or weights on inversion.

3.2. *Parameter sensitivity*

The initial and final parameter sensitivities of the nine runs are shown in Fig. 3. The initial and final parameter sensitivities were calculated using Eq. (2) at the beginning and end of the optimization processes (i.e., Eq. (1)). Although the final sensitivity is more important, comparing these two sensitivities can suggest how parameter sensitivities have changed during the inversion process at individual sites and how these changes behave across sites. A consistent change pattern of parameter sensitivity across sites would suggest that observations had a similar impact on resolving model parameters across these sites. DEC11 was optimized in Run1 to Run4 (Fig. 3a–d and i–l). It had the lowest sensitivity among all the optimized parameters except its final sensitivity in Run4 (Fig. 3l). This suggests that DEC11 could not be resolved by the available field data when the number of optimized parameters was more than 3. DECW1 had the second lowest sensitivity among all the optimized parameters in Run1 and Run2 (Fig. 3e–h), although its sensitivities were relatively high initially in Run2 (Fig. 3g). Run3 further proved that the available field data contained little information to determine DECW1.

Other parameters including DEC4, PRDX4, WOODDR2, and TEFF2 had relatively high sensitivities, indicating that the field observations contained more information about these parameters. These results indicated that the available field data could resolve three parameters reasonably well at the same time.

Fig. 3 also shows that parameter sensitivities varied among sites and life zones. In all runs except Run7 and Run8 (which were not successful, see Section 3.5), parameter sensitivities were lower in tropical dry and moist life zones, likely indicat-

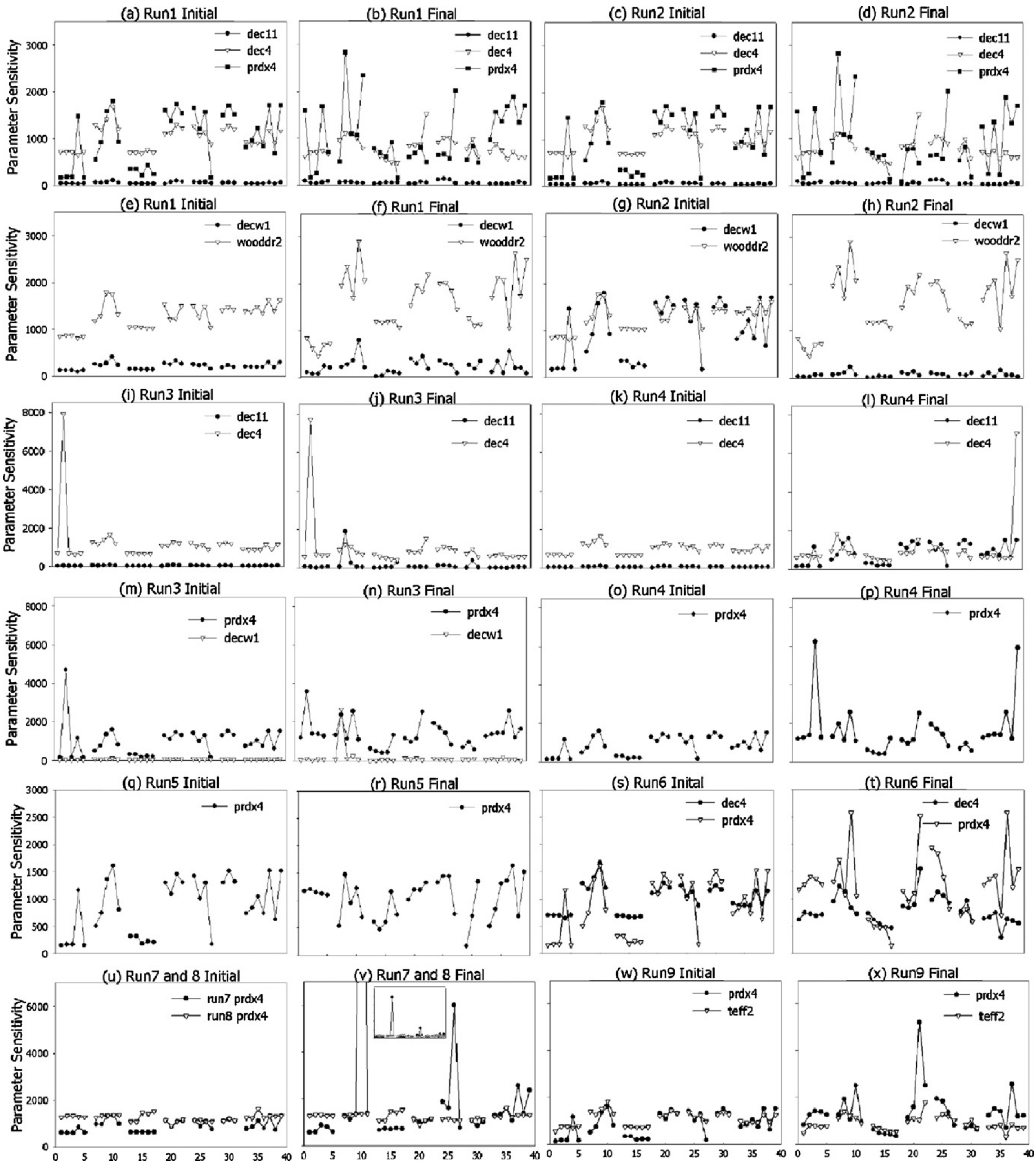

Fig. 3 – Initial and final parameter sensitivities of the optimized parameters for all model runs at the 39 sites.

ing that field data collected in these two life zones contained less information about these parameters than in other life zones. This might also suggest that CENTURY model is more applicable to other life zones. The variability of parameter sensitivities among sites suggests that the available data resolved optimized parameters differently. This seems hard to explain because the number and meanings of observations were the same for all the sites. This variability might reflect the adaptability of the model to different sets of field measurements via adjusting these optimized parameters.

3.3. *Parameter correlation coefficients*

Fig. 4 shows the correlation coefficients between adjustable parameters for all the model runs that had multiple adjustable parameters. Run5, Run7, and Run8 had no correlation coef-

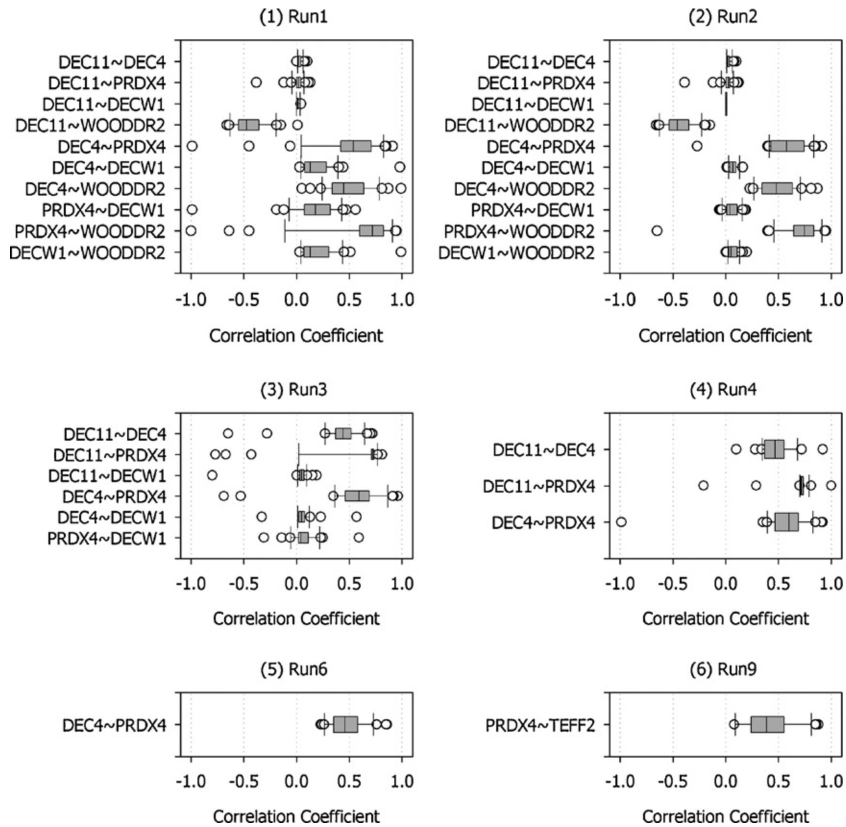

Fig. 4 – Variability of parameter correlation coefficients across sites and model runs.

ficient because only one parameter was adjustable during each of the runs. It can be seen from Fig. 4 that parameter correlation coefficients of the same two parameters varied from site to site and from run to run. The parameter correlation coefficients of Run1 were similar to those of Run2 with the highest correlation values between the following sets of parameters: PRDX4 and WOODDR2, DEC4 and PRDX4, and DEC4 and WOODDR2. DEC11 had very low correlation coefficients with DEC4, PRDX4, and DECW1. DEC11 was negatively correlated with WOODDR2, which was the only consistently negative correlation found among all the parameters during all model runs.

DEC11 became correlated with DEC4 and PRDX4 during Run3 and Run4 (Fig. 4(3) and (4)). DECW1 was not correlated with any other adjustable parameter (i.e., DEC11, DEC4, or PRDX4) in Run3. DEC4 and PRDX4 were correlated during Run3, Run4, and Run6.

Note that the some parameter correlation coefficients were very different from the normal in terms of their magnitudes and the directions (positive or negative) of correlation. For example, the correlation coefficient between DEC4 and PRDX4 had only three negative values out of a total of 39 possible values during Run1 (Fig. 4(1)). A total of 12 site-runs (out of 198 site-runs or 6 percent of the total) had generated correlation coefficient outliers. These site-runs were:

Run1: Meseta, Pacifica3, Bonita, Gallo Pinto, and Magsassy.
Run2: Meseta, Pacifica3, and Bonita.
Run3: Pacifica1, Nubosa, and Osa3.
Run4: Osa3.

According to Poeter and Hill (1998), a correlation coefficient larger than 0.90 suggests that the parameters are correlated, and hence the values of parameters would be highly uncertain. No single pair of parameters was consistently correlated (i.e., correlation coefficient >0.90 for all sites and all runs). Just a few sites had correlation coefficients higher than 0.90. Correlation coefficient outliers might indicate that the model was difficult when applied to some sites in tropical wet and tropical dry life zones.

3.4. *Parameter uncertainty*

Fig. 5 shows the optimized parameter values and their corresponding 95% linear confidence intervals. Results suggested that the confidence intervals of DEC11 (Fig. 5A1–A4) and DECW1 (Fig. 5F1–F3) were consistently wider than other parameters' across all the model runs and all the sites. The confidence intervals of PRDX4 varied among model runs (Fig. 5D1–D9) with the smallest intervals for runs with 2–4 optimized parameters (Run3, Run4, Run6, and Run9), intermediate intervals for runs with 5 optimized parameters (Run1 and Run2), and wider intervals for runs with only one optimized parameters (Run5, Run7, and Run8).

Large confidence intervals of DEC11 and DECW1 agreed with the observations from parameter sensitivities that these

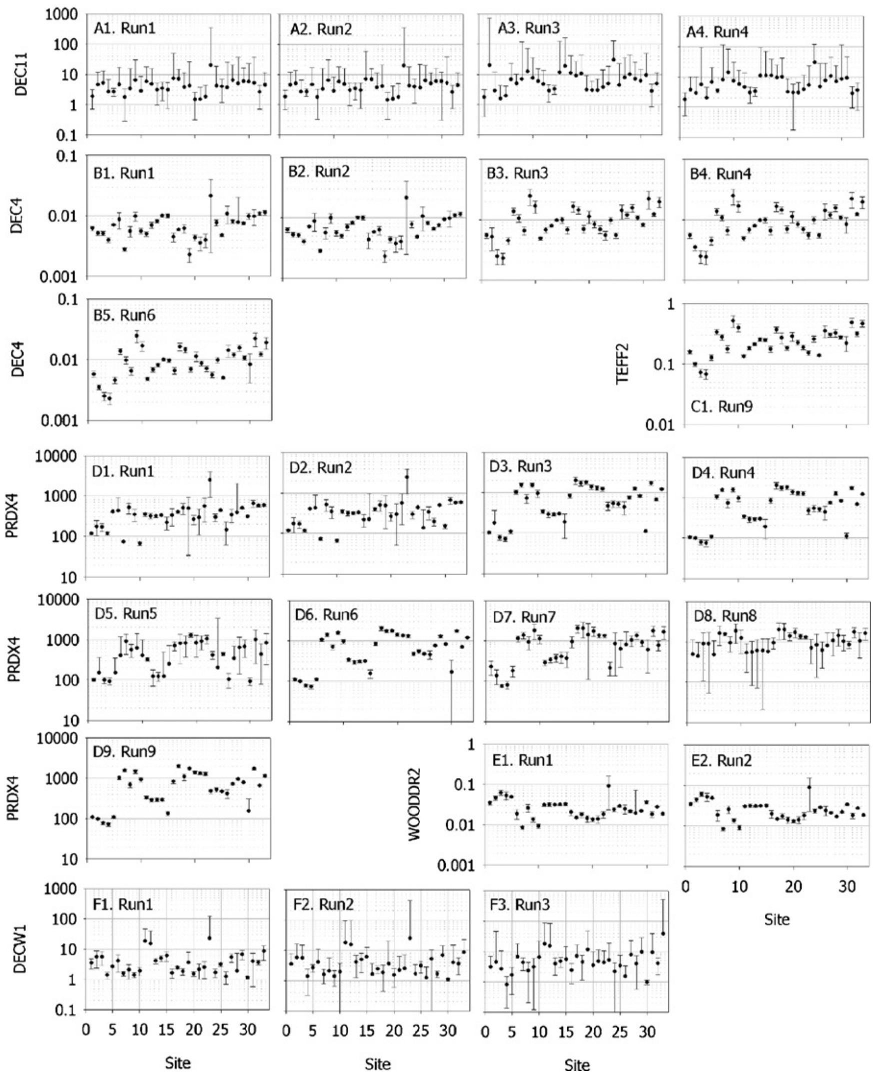

Fig. 5 – Parameter uncertainty.

two parameters were relatively insensitive because limited information was contained in the observations about these two parameters. This suggests that both over- and under-fitting are likely to increase the uncertainty of parameter values for a given set of observations. All other parameters were well resolved as suggested by their small confidence intervals. In general, DEC4 is better resolved than any other parameters.

3.5. *Goodness of model fit across sites*

Detailed comparisons between simulated and observed values, along with the results of significance test on their difference (indicated by the background), for all 9 model runs across the 39 sites are presented in Fig. 6. It shows the following results:

1. A total of 50 (out of 81) comparisons showed that the simulated values were significantly different from observations.
2. The simulated LITTERN and WOODN were significantly lower than observations, which was consistent across all model runs.
3. All simulations were significantly different from their corresponding observations for all the variables in Run7 and Run8.
4. Except Run1 and Run2, no relationship existed between the simulated and MODIS NPP values. MODIS NPP values were compressed to a narrow range as compared with the simulated values.
5. The number of matches between simulated and observed values increased with the increasing number of adjustable parameters.
6. Among all nine variables, simulated ABGC, SOMTC, and SOMTN values agreed with observed values in more model runs than other variables.
7. CENTURY model was more robust in simulating C dynamics that N dynamics. CENTURY completely failed the simulation of LITTERN and WOODN, although the corresponding simulation of LITTERC and WOODC were

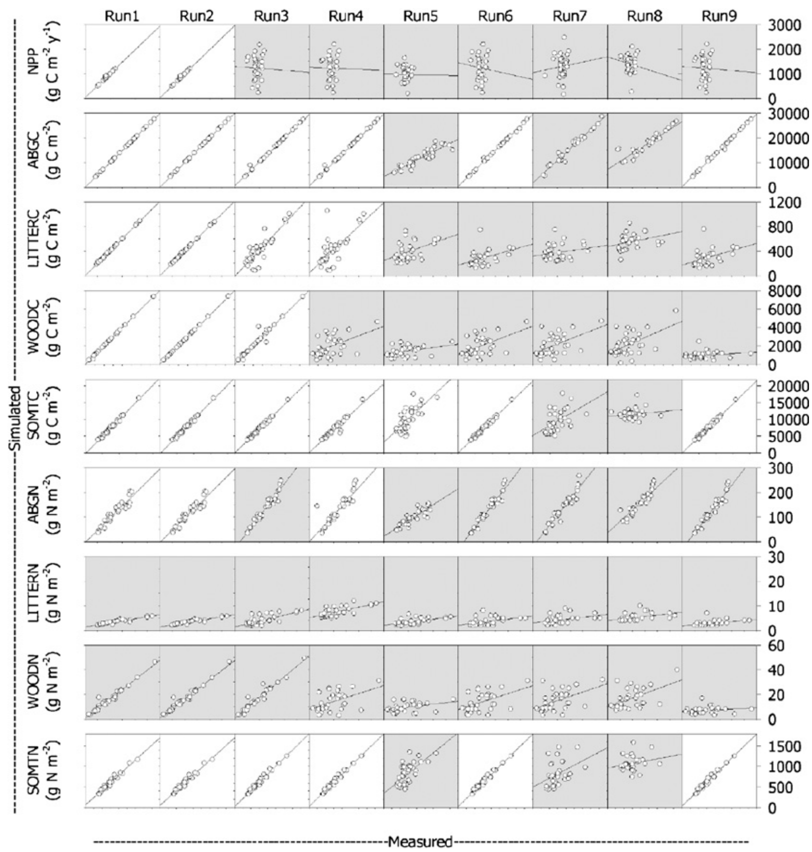

Fig. 6 – Goodness of model fit as demonstrated by the comparison between simulated and measured values for the 9 model runs across 33 sites. A successful model fit (white background) indicates that (1) the model explained a significant portion of the variability of field observations, (2) the slope of the linear regression between observed and simulated values was not significantly different from 1.0, and (3) the intercept of the linear regression was not significantly different from 0. Failing any of these significance test criteria suggests a failed model fit (grey background).

successful in some runs. The simulation of ABGC was also better than that of ABGN.

3.6. *Parameter modeling*

Not surprisingly, the best Cubist parameter models, indicated by the best correlation coefficients and the lowest relative errors, were produced when all the site and parameter variables were possible independent variables. However, these were not the best practical set of models since all of the parameters depended on one or more of the other parameters to be derived. Because the goal was to be able to derive all of the parameters from known data, models using only site factors (e.g., temperature and precipitation) had to be used for some parameters. Highest correlation coefficients and lowest relative errors were not sufficient to select models, and precedence in the prediction of parameters has to be considered simultaneously. The precedence of the six variables is shown in Fig. 7 and Table 5. From Fig. 7, it can be seen that because dec11 depended on dec4 that depended on dec5, it is necessary to estimate dec5 first. This suggests that they have the following precedence: dec5, dec4, and dec11. The predictive models for dec4 and dec5 were as follows:

dec4:

$$\text{dec4} = -0.01023 + 0.045\,\text{dec5}$$

dec5 (committee model):

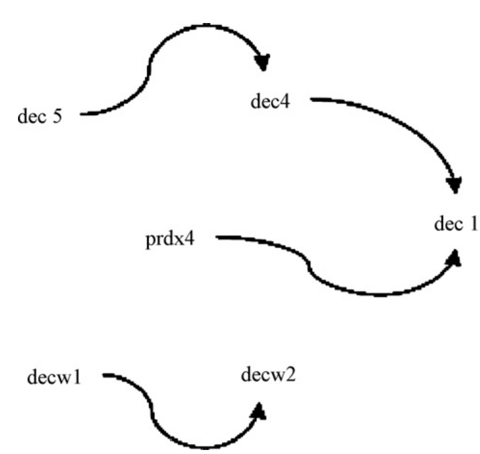

Fig. 7 – Dependence and precedence for generating parameter fields.

Table 5 – Model type, precedence, correlation coefficient, and relative error for each of the regression tree models

Target variable	Best practical Cubist model	Precedence	Correlation coefficient	Relative error
dec5	Committee model	1	0.83	0.58
dec4	Committee model	2	0.98	0.13
decw1	Single rule model	1	0.95	0.41
decw2	Single rule model	2	1.00	0.00
prdx4	Single rule model	1	0.84	0.47
dec11	Committee model	3	0.68	0.77

Model 1:

$$\text{dec5} = 2.574 - 0.107\,t_{\text{min}} - 0.000266\,\text{elevation}$$

Model 2:

$$\text{dec5} = -0.132 + 0.000185\,\text{precipitiaton}$$

Model 3:

Rule 1: If lifezone is T-df, P-wf, T-mf, P-rf

$$\text{dec5} = 0.555 - 0.067\,t_{\text{min}} + 0.036\,t_{\text{max}}$$

Rule 2: If lifezone is T-wf, LM-rf

$$\text{dec5} = 0.987 - 0.09\,t_{\text{min}} - 0.048\,t_{\text{max}}$$

Model 4:

$$\text{dec5} = 3.529 - 0.152\,t_{\text{min}} - 0.00048\,\text{elevation}$$

Model 5:

Rule 1: If lifezone is T-df, P-wf, T-mf, P-rf

$$\text{dec5} = -0.75 + 0.000147\,\text{prec} + 0.033\,t_{\text{min}}$$

Rule 2: If lifezone is T-wf, LM-rf

$$\text{dec5} = 0.741$$

Model 6:

$$\text{dec5} = 3.586 - 0.158\,t_{\text{min}} - 0.000397\,\text{elevation}$$

Model 7:

If lifezone is T-df, P-wf, P-rf

$$\text{dec5} = 0.215$$

If lifezone is T-wf, LM-rf, T-mf

$$\text{dec5} = 0.544 - 0.191\,t_{\text{mean}} + 0.161\,t_{\text{max}}$$

The units of the independent variables were: precipitation in mm y^{-1}, t_{mean}, t_{min} and t_{max} in °C, and elevation in m above sea level.

4. Discussion

The agreement between simulated and observed values increased with the increasing number of adjustable parameters n. This is consistent with the general trend that a perfect fit can always be reached by increasing n as a result of over-fitting. In this study, the maximum n used was 5 (i.e., Run1 and Run2), resulting in the highest agreement between simulated and observed values. Although the fitting of LITTERN and WOODN was unsuccessful in these two runs, simulated values of other variables matched very closely with observations. We believe that n with a value of 5 has already resulted in over-fitting some observations, notably MODIS NPP (Fig. 6). Most of the simulated NPP values in Run3 through Run9 varied from 500 to 2000 g C m^{-2} y^{-1}, comparable with field observations in the tropics (Clark et al., 2001). In contrast, MODIS NPP values were compressed around 700–1100 g C m^{-2} y^{-1}. The over-fitting of NPP in Run1 and Run2 does not mean all the observations had been over-fitted. In fact, LITTERN and WOODN were still poorly fitted. The coexistence of over- and under-fitting in Run1 and Run2 might be caused by the deficiency of the CENTURY model, failure to include sensitive parameters related to LITTERN and WOODN, or incorrect weights assigned to the observations.

Under-fitting can happen if there are not enough adjustable parameters as demonstrated by Run5, Run7, and Run8. These runs suggest that adjusting PRDX4 and its tied parameters was not enough to take advantage of the information contained in the observations. The failure of tying decomposition coefficients (e.g., DEC11, DEC4, and DEC5) to PRDX4 to explain the variances in observations also suggested that the spatial variations of DEC11, DEC4, and DEC5 were not well coupled with production. Furthermore, Run5 indicated that these decomposition coefficients, treated as constants in fix.100 of CENTURY, should not be treated as invariants.

CENTURY successfully simulated ABGC, SOMTC, and SOMTN, when the number of adjustable parameters was larger than 1. This is very encouraging because the main focus of this research is to investigate the capability of CENTURY model in simulating ABGC and SOMTC by adjusting model parameters. CENTURY simulates SOMTC better than any other N pools which might reflect the fact that the model was originally developed for agricultural systems with a special emphasis on the characterization of soil biogeochemical processes. The better performance of the model on ABGC, SOMTC, and SOMTN was consistent with the high observation sensitivities of these variables (Fig. 3). This suggests that these observations not only contribute more information to the parameter estimation process, but they can be better predicted as well.

Our results showed that the values of 2–4 parameters could be successfully resolved with the available information. Under-fitting could be resulted from only one adjustable parameter, which led to a failure of comparison between simulated and observed values. Adjusting more than four variables could result in over-fitting at least partially. At the same time, the mismatches between the observed and simulated nitrogen stocks (i.e., LITTERN and WOODN) suggest that we might have ignored some parameters controlling nitrogen dynamics in the model. The values of one or two of such parameters might be resolvable. Some observations including MODIS

NPP and LITTERNN contained little information that helps to resolve parameter values. However, this information did provide evidence of over-fitting once the number of adjustable parameters exceeded 5.

Almost a perfect match of ABGC is worrisome because field measurements are snapshots which might well be different from the long-term averages. Higher temporal variability of ABGC might partially explain why the sensitivities of SOMTC and SOMTN were comparable or higher than that of ABGC, or in other words, the information content of SOMTC and SOMTN was equivalent or higher than that of ABGC. SOMTC and SOMTN pools are more stable than ABGC pools. Therefore, they might contain more information about the steady state conditions than the more variable ABGC.

Weights are necessary when different kinds of observations are used in the cost function. Various methods have been used to assign weights to observations, including the inversion of standard deviation (ISD) (Poeter and Hill, 1998), the inverse of the mean observation value (IMO) (Poeter and Hill, 1998), or expert knowledge. All these methods have their advantages and drawbacks. The first two methods are objective and can be quantified. However, both of them might not reflect the quality and importance of observations at the same time. For example, the high sporadic temporal variation (at the decadal scale) of coarse woody debris (CWD) on a given forest site dictated that a relative low weight should be placed in the one-time measurement of CWD in the parameter optimization process. The ISD method will likely reflect the low confidence in this kind of sparse CWD measurements correctly, while the IMO will not. However, the ISD method will not reflect the increase of confidence in data quality as the number of CWD measurements increases. The IMO simply assigns weights according to the magnitude of the observation, which implicitly assumes that the quality of the various kinds of observations is the same. In reality, this assumption might not be met all the time. For example, in this study, the magnitude of CWD (i.e., WOODC) was similar to that of soil organic carbon in the top 20-cm soil layer (i.e., SOMTC) at some sites. Assigning equal weights to these observations would be unjustifiable because the temporal variability of SOMTC for a given site is much smaller than that of WOODC, which suggests a larger weight should be assigned to SOMTC to reflect that it more likely represents the long-term steady state SOMTC conditions. Another factor that the IMO and ISD methods do not reflect well is the relative importance of different observations for a given application. In practice, higher importance usually calls for a larger weight. We believe that the importance of total aboveground biomass carbon (i.e., ABGC) is much higher than the importance of litter (i.e., LITTERC) given that our overall objective is to assess the capability of the model in simulating total carbon at the ecosystem level. However, if the purpose were to evaluate the overall performance of the model in simulating various processes and entities, assigning weights using the ISD and IMO methods would be appropriate.

Fig. 8 shows the comparison between the NPP values inversed from Run3 (Runs 3–6 and 9 had similar results) with those derived from field measurements in the tropics along precipitation and temperature gradients. Our inverse values seem demonstrated some interesting patterns that were different from field observations. For example, higher temperature usually is associated with lower precipitation (i.e., the dry tropical forest life zone), resulting lower NPP. Meanwhile, NPP was around its maximum with a mean annual temperature of 20 °C and annual precipitation of 3500–4000 mm. In contrast, the NPP values derived from field measurements as shown in Clark et al. (2001) indicated that the NPP values were the lowest when annual temperature was around 20 °C. Biologically, this is possible if these sites had water limitations. However, the NPP values derived from field measurements by no means captured the entire spectrum of possible NPP values along the precipitation and temperature gradients, which is indicated by the NPP values inversed from this study. When plant growth is not limited by precipitation or other factors, NPP values should not be the lowest around 20 °C because this temperature is close to the optimal temperature for plant growth. Although the model inversion technique can be used to possibly advance our understanding of NPP, the NPP results and their relationships with precipitation and temperature presented in this paper deserve more studies in the future.

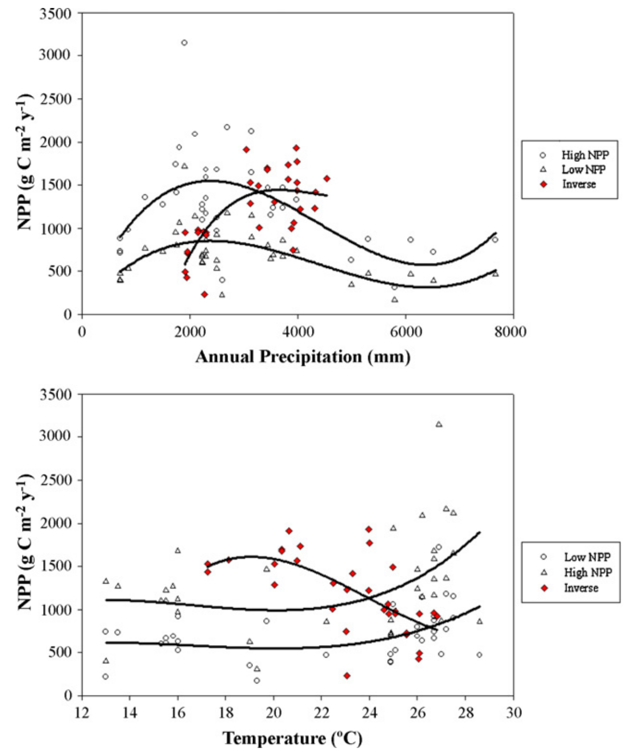

Fig. 8 – Comparison of NPP inferred from model inversion (Run3) with estimates from field measurements. Low and high NPP estimates were from Clark et al. (2001).

This study demonstrates that some model parameter values can be resolved, and the key carbon flux NPP at the ecosystem level can be inferred from C and N stock measurements using nonlinear model inversion. To our knowledge, C and N stock measurements have not been utilized in this context before. The results of this study have several important implications. First, this method might be very useful to derive model parameter and NPP values from C stock measurements from mature forests in the world that have already been acquired by national to regional forest inventory systems. Second, because of the difficulties involved in the estimation of NPP using observational approaches (Clark et al., 2001) and its importance in the carbon cycle, the ability of inferring NPP values from C stock measurements in mature forests can contribute significantly to our understanding of the global to regional carbon cycle. The NPP databases generated using this approach can be used to improve the calibration and validation of NPP algorithms, and therefore potentially enhance our capability and accuracy of predicting NPP using remote sensing technologies. Third, the optimized parameter values can be analyzed to develop predictive relationships with site conditions such as precipitation and temperature as well as other parameters (i.e., correlation). Parameter surfaces can then be generated from these predictive relationships to support the deployment of the model in space.

Although the proposed approach takes a model at face value and parametric evaluations are limited to model (CENTURY) formulation, it is capable of detecting deficiencies in model formulations. For example, a good formulation should render the model parameters independent of climate. However, this study shows that some of the CENTURY parameters depend on climate, suggesting more work should be done to reformulate that part of the CENTURY model. Another weak component of the CENTURY model (and many others like it) is that many of the parameters are fundamentally correlated with one another. The approach reveals the degree of parametric inter-connectedness. While attempts can be made with rules to overcome some of this problem, ultimate solutions would be to modify the original model formulation and related assumptions according to the new understanding.

5. Summary

Traditionally, only carbon fluxes have been used to infer model parameter values using nonlinear inversion or data assimilation techniques. In this study, we successfully inferred model parameter values using field observations of C and N stocks collected from tropical mature forests with the assumption that C and N stocks in these forests have reached equilibrium conditions. Results clearly indicated that these measurements can resolve a certain number of model parameters without under- or over-fitting. That the information contents varied among field measurements can be used to prioritize the field sampling strategies to maximize the total information return from field campaign.

The inversed values of model parameters can be further analyzed, and predictive models of these parameters can be developed to facilitate the spatial deployment of plot-scale models in regional model simulations. However, inter-dependency among parameters needs to be addressed using precedence rules. Developing parameter fields will likely play an increasing role in landscape to global model simulations.

Inversed NPP values from this study revealed that previous NPP estimates derived from field measurements in the tropics might not represent the whole of spatial variability of NPP, as indicated by the different NPP patterns along the precipitation and temperature gradients. Although the NPP values inversed from this study make biological sense, a more objective verification with NPP derived from field measurements should be conducted in the future. If the verification is successful, NPP values could be inferred from many mature forests in the world that are monitored by national to regional forest inventory systems.

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